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Published in:
Chemistry Central Journal

DOI:
10.1186/1752-153X-3-S1-P57

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2009

Link to publication in University of Groningen/UMCG research database

Citation for published version (APA):
Baum, I., Haller, L. A., Schwab, L. W., Loos, K., & Fels, G. (2009). Molecular modeling studies of lipase-catalyzed β-lactam polymerization. *Chemistry Central Journal*, *3*, [P57]. https://doi.org/10.1186/1752-153X-3-S1-P57

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Chemistry Central Journal

Poster presentation

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Molecular modeling studies of lipase-catalyzed β-lactam polymerization

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from 4th German Conference on Chemoinformatics
Goslar, Germany. 9–11 November 2008

Published: 5 June 2009

Chemistry Central Journal 2009, **3**(Suppl 1):P57 doi:10.1186/1752-153X-3-S1-P57

This abstract is available from: http://www.journal.chemistrycentral.com/content/3/S1/P57

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Enzymatic polymerization has emerged over the last 5 years as a field of considerable interest and commercial promise. The reaction proceeds with high regio-, enantio-, and chemoselectivity under relatively mild conditions. Enzymes have been used so far to synthesize polyesters, polysaccharides, polycarbonates, polyphenols, polyanilines, vinyl polymers, and poly-amino acids [1]. Particularly, lipase B of *Candida antarctica* immobilized on polyacrylic resin (Novozyme 435) has proven to be a very versatile catalyst and has successfully been used for the synthesis of polyesters from various substrates [2][3][4]. Little, however, has been reported on the enzyme catalyzed synthesis of polyamides [5].

While it has been shown that nylons can chemically be produced from the corresponding amino acids or by anionic ring-opening polymerization of 5–13 membered unsubstituted lactams, poly-β-alanine has not yet been obtained by either polymerization of β-alanine or β-lactam (2-azetidinone). Using lipase B of *Candida antarctica* we have recently been successful in the production of unbranched poly-βalanine starting from unsubstituted β-lactam [6].

Here we report preliminary molecular modeling studies of the lipase catalyzed ringopening polymerization of β-lactam towards an understanding of the underlying enzymatic mechanism. We can show that amide formation initially follows the well-known enzymatic acylation of Ser105 by β-lactam using Asp187 and His224 of the catalytic centre and Thr40 and Gly106 as oxy-anion hole. The elongation of the chain, however, utilizes different parts of the active site. The mechanism is only applicable for β-lactam and can not be utilized by β-alanine and suggests a reasoning for the experimental finding that β-alanine can not be polymerized enzymatically but rather inhibits the polymerization in a copolymerization experiment with β-lactam and β-alanine.

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